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Chapter

Numerical and Experimental Analysis of Thermochemical Treatment for the Liquefaction of Lemon Bagasse in a Jacketed Vessel

Brenno S. Leite, Daniel J.O. Ferreira, Sibele A.F. Leite and Vanessa F.C. Lins

Abstract

In this work, it was investigated the time evolution of thermal profile inside a liquefaction vessel and how the temperature and time of reaction influenced liquefaction yield. Liquefaction was performed in two different ways: (1) Experimental Analysis; (2) Numerical 3-D model, using Computational Fluid Dynamics (CFD). Liquefaction was performed using lemon bagasse samples, glycerol and sulphuric acid, as catalyst. Temperature and liquefaction Yield (LY) were measured for different time of reaction (30, 60 and 90 minutes). From experimental data, LY were higher than 70 wt% for 90 minutes reaction. The increase in the temperature inside the reactor occurred due to the conduction and natural convection phenomena. Although the jacketed vessel was fed with steam at 125°C, working conditions allowed the heating of the mixture to less than 100°C. CFD thermal profile was in accordance with experimental data. They showed it was necessary 60 minutes to achieve a steady state of heating in the mixture inside this liquefaction vessel. From CFD transient simulations, it was observed some oscillations and detachment from experimental data, which may be due to changes in fluids properties along the process. Despite this consideration CFD could satisfactory analyse heat transfer in this liquefaction process.

Keywords: biomass, polyol, CFD, liquefaction yield, glycerol

1. Introduction

The use of biomass and agricultural waste as an alternative to fossil products has been widely investigated in the last decades. Several processes have been developed to provide more efficient use of those renewable sources and generate the so-called "green products", with properties and performance comparable to petroleum derivative products [1]. Polyol is one of these potential green products, since it is an essential polymer in the polyurethane compounds industry. It may produce foams, elastomers, inks, paints and others, which are currently obtained from petroleum derivatives.

A "green polyol" can be obtained from biomass liquefaction process [2]. This process consists of the endothermic reaction between biomass, solvent and catalytic agent, followed by an exothermic recombination of molecules, during a specific time interval. Biomass liquefaction is usually carried out in a jacketed reactor, that can be a stirred tank or a single vessel, without mechanical stirring [3].

The liquefaction yield depends on the technology used to modify the structure of the lignocellulosic biomass and the raw material. Because of the importance of the temperature on liquefaction process, some works performed an investigation of liquefaction yield and polyol properties as a function of temperature and time reaction [2, 4–6].

According to earlier literature, a wide range of temperature have been used on liquefaction processes. Dimitriadis and Bezergianni [7] reported a temperature range between 200–450°C (473.15–723.15 K) for the hydrothermal liquefaction, which varied according to the solvent, the biomass and the process used. Rafiqul [8] set autoclave temperature around 350–450°C (623.15–723.15 K) to perform co-liquefaction of bituminous coal with bagasse. To liquefy rice straw, using glycerol as solvent, Cao [9] used autoclave, with thermopar probes, set in the temperature between 220–300°C (493.15–573.15 K). Ye [2] evaluated the liquefaction process, of bamboo shoot with two types of glycerol, using heat and stirring. In this study, temperature varied around 110–150°C (383.15–423.15 K) with the best liquefaction yield at 150°C. Also, there was no significant difference on liquefaction yield, after 80 minutes of reaction (2). Li [10] investigated the liquefaction of wheat straw using alcohol/water mixed solvent. They observed better results for liquefaction yield at 270°C (543.15 K), using a residence time lower than 120 minutes.

Despite the significant importance of the temperature and time on the liquefaction process, it is still necessary to set a method to help researches choose these operational parameters. As shown in this review, it has been seen considerable variation among temperatures values and its range. Therefore, a suitable analysis of the heat transfer would be an interesting tool for industrial and academic applications to understand temperature and time reaction, in the liquefaction process.

Hence, in this work, the time evolution of thermal profile inside the liquefaction vessel and how temperature and time of reaction influenced liquefaction yield were investigated. Based on the above considerations, the analysis of liquefaction was performed in two different ways:

1. Experimental Analysis: the liquefaction of lemon bagasse with crude glycerol, to produce polyol, was conducted in a heated jacket reactor, supplied by steam, at constant values of temperature and pressure.

2. Numerical 3-D model: Computational Fluid Dynamics (CFD) was used considering two computational domains. The first domain considered the fluid flow of superheated steam inside the heated jacket at steady state flow rate. The second domain represented natural convection of glycerol and lemon bagasse mixture (polyol) considering transient fluid motion.

The experimental and numerical results were compared in order to validate the CFD simulation. It is expected that the simulation could be a helpful tool to evaluate velocity and temperature profiles for transient and steady state operations in further liquefaction experiments, despite geometries and scales used. In this way, it may guide researches choose temperatures and time reaction, in order to have better liquefaction yield with lower energy consumption.

2. Materials and methods

2.1 Materials

Lemon bagasse samples were collected between May and October of 2016 in the southeast region of Brazil (19° 53′ 12″ - S; 44° 25′ 56″ - W). The samples were dried at 105°C using an oven-dry, until a constant weight was achieved. Then, the biomass was cut in a knife mill to get fibbers of 0.5 mm length. The crude glycerol, used as liquefaction solvent, was kindly provided by Petrobrás (Usina Darcy Ribeiro - Montes Claros - MG, Brazil). Sulphuric acid (Synth) was used as catalyst for this reaction.

2.2 Experimental analysis

The experiments were performed in a jacket vessel. The reactor was supplied with a mixture of lemon bagasse (biomass), crude glycerol (solvent) and a sulphuric acid solution (95 wt%), as catalyst [11]. The steam used to feed the reactor was produced in an autoclave (water steam at 125°C - 398.15 K). The reaction was performed using three length of time: 30, 60 and 90 minutes. The experimental parameters: temperature, pressure, time and catalyst, have significant impact on the liquefaction process [5, 12]. Hence, in the present work, length of time reaction was investigated for three different solvent/biomass ratio. The solvent/biomass ratio conditions and their respective obtained Polyol are shown in **Table 1**.

From the reaction, it was produced a mixture of polyol and residues. Each resulting mixture was filtered to separate the two components: polyol and solid residues. The solid residues were dehydrated at 75°C (348.15 K), for 72 hours, to calculate the liquefaction yield (LY), obtained in weight percentage (wt%) as shown in Eq. (1) [8, 12]:

$$LY = \left(\frac{\text{Biomass weight} - \text{Residue weight}}{\text{Biomass weight}} \right) \cdot 100 \qquad (1)$$

Where the biomass weight is the lemon bagasse weight (g) and the residue weight is the insoluble lemon weight, after the liquefaction process (g). The higher the LY, the higher is the polyol production.

2.3 Analysis of heat transfer

The temperatures in the centre of liquefaction vessel were recorded by a thermopar probe Digital Thermometer model K-type-1-channel brand Thermocouple Thermometer. It was done for 90 minutes, in time intervals of 5 minutes,

Variables	**Mixture para obtenção do poliol**		
	Polyol 1	**Polyol 2**	**Polyol 3**
Ratio solvent/biomass (wt%)	2:1	3.5:1	5:1
Lemon Bagasse (g)	115.00	78.00	58.00
Glycerol (g)	230.00	273.00	290.00
Suphuric Acid (g)	7.00	7.00	7.00

Table 1.
Liquefaction variables used to obtain the polyols.

considering the three solvent/biomass ratios presented (Polyol 1, 2 and 3). Temperature probes were located inside the reactor: one at the centre of the axis and another at the centre of the bottom. Data obtained was used to compare with CFD results.

The temperature data collections were performed at intervals of the $\Delta t = 5$ minutes, considering the initial temperature Ti = 25°C (298.15 K). Temperature variations (ΔT) and final temperature (Tf) were measured for each experimental run according to their respective intervals of time (0-30 minutes, 30-60 minutes, 60-90 minutes).

2.4 Reactor configurations

The jacketed reactor used in the present work is made of stainless steel and its geometry is showed in **Figure 1**.

The dimensions presented in **Figure 1** are: (a) jacket internal radius: 56,5 mm, (b) jacket external radius: 76,5 mm, (c) diameter of the input and output for steam in the jacketed: 20,0 mm, (d) thickness of the heat transfer surface: 2,0 mm, (e) total height of the reactor: 220 mm, (f) internal height of the reactor: 200 mm and (g) diameter of the steam input: 25,4 mm.

2.5 Numerical 3-D CFD model from

The Computational Fluid Dynamics (CFD) is a numerical technique used to solve fluid flow problems described by transport equations for mass, energy and momentum conservations employing the Finite Volume Methods (FVM) in three dimensional geometries. In the present CFD simulations, it was assumed that the internal shell thickness, between the steam and polyol domains, is negligible compared to dimensions of the heated jacket and liquefaction. The thermal resistance of the liquefaction vessel shell can be assumed negligible due to its high conductivity of the stainless steel compared to steam and glycerol mixture. It was also assumed constant temperature at the top surface of the vessel in the polyol domain and external adiabatic walls in the jacket domain. Each case was composed by two different simulations:

i. a steady state analysis for steam at 125°C flow passing through the jacket domain;

ii. a transient analysis of the natural convection of the polyol mixture inside the reactor vessel domain, heated by external walls which heat transfer is function of the wall heat transfer coefficient imported from jacket domain results.

The geometry of the reactor domain must fit perfectly inside the internal cylindrical hole of the jacket domain. Therefore, the reactor domain and the internal cylinder of the heat jacket have 200 mm height and 113 mm diameter. The computational mesh used for the liquefaction vessel domain for jacket domain were composed by 2,504,216 structured cells and 1,0763,346 non-structured cells, respectively.

Since it was not expected that temperature variations inside liquefaction vessel can perturb the thermal profile of the jacket domain, it was assumed one-way "communication" between the two computational domains. The results from jacket domain were used as boundary condition of wall heat transfer coefficient for polyol domain simulations. In the jacket domain the fluid employed was Water Vapor at 100 °C, available

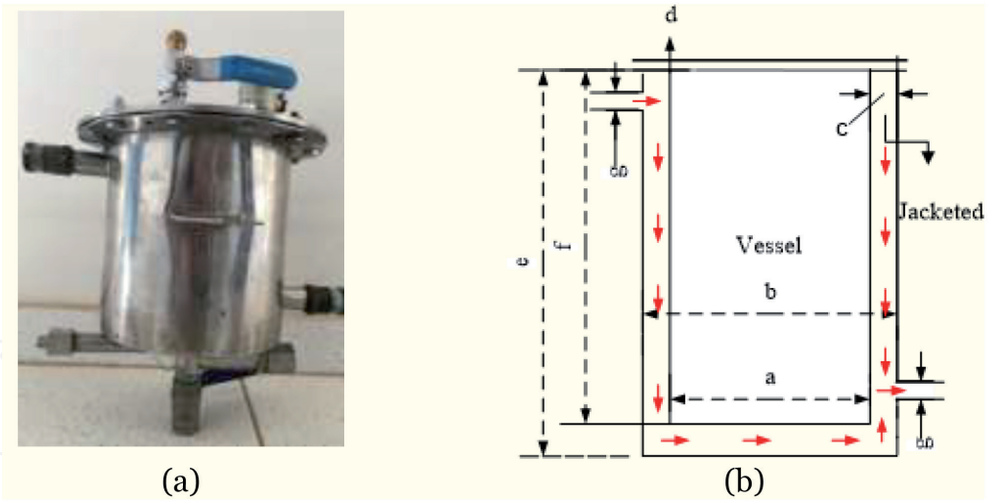

Figure 1.
The reactor model: (a) Jacketed reactor; (b) the geometry of reactor (values expressed in mm), red arrows represent water vapor flux.

Domain jacket			**Domain reactor**		
Fluid	**Water vapor at 100°C**	**Fluids**	**Polyol 1; 2 and 3**		
Simul. type	Steady state	Simul. type	Transient 90 min time-step: 0.1 s max. iter. per t-s: 40 convergence per t-s: 10-4		
Turbulence	SST (5%)	Turbulence	Laminar, SST (5 %)		
Heat transfer	Thermal energy	Heat transfer	Thermal energy		
		Buoyancy	g [m/s^2] = (0.00; -9.81; 0.00)		
Boundary conditions			**Boundary conditions**		
Inlet	0.01 kg/s; 125°C	External wall	Imported wall heat transfer coeff. profile with ext. 125°C		
Outlet	0.01 kg/s	bottom walls			
Internal walls	Fixed temp. 25°C	upper wall	Fixed temp. 25°C		
External walls	Adiabatic	Initial temp.	25°C		
Fluid physical properties					
Parameter	**Glycerol**	**Lemon Bagasse**	**Polyol 1**	**Polyol 2**	**Polyol 3**
ρ [kg/m^3]	1260.0	1300.0	1273.2	1268.8	1266.8
ν [kg/(m.s)]	1.4800	1.5000	1.4866	1.4866	1.4866
k[1] [W/m.K]	0.29	0.061	0.2102	0.2352	0.2465
cp[2] [J/kg.K]	2428.0	2825.52	2559.2	2515.5	2495.6

[1][13].
[2][14].

Table 2.
Physical properties, configurations, simulation parameters and boundary conditions employed in the superheated steam flow and natural convection simulations of jacket and polyol domains.

in the library of Ansys CFX software. In order to analyse the heat transfer inside the reaction vessel, it was assumed ideal mixture of glycerol and lemon bagasse for the following physical properties: density, viscosity, thermal conductivity and specific

heat capacity. The transient natural convection simulation for biomass liquefaction used single-phase fluids.

The physical properties were estimated by data for the three solvent/biomass rates: 2:1, 3.5:1, 5:1, whose cases are denominated Polyol 1, Polyol 2 and Polyol 3, respectively. In the reactor domain, the flow was assumed laminar due to the motion of the glycerol mixture (promoted by natural convection), which is characterized by low values of Ra and Nu inside the liquefaction vessel. In the jacket domain, it was considered turbulent flow represented by the SST (Shear Stress Transport) model. It is a RANS (Reynolds Averaged Navier Stokes) model that considers isotropic velocities fluctuations in the fluid flow. Despite of the low Re values, which is an evidence of laminar flow, it was expected the formation of three dimensional natural convection cells that evaluates in time, which are characteristic of turbulent flows. Therefore, for the polyol domain simulations, it was performed two runs of CFD simulations for each case, considering laminar and turbulent (SST model) flow, respectively. The simulation time was 90 minutes with time-step of 0.1 seconds and 40 iterations for each time-step. The fluid physical properties such as specific mass (ρ), cinematic viscosity (v), thermal conductivity (k) and calorific capacity (c_p) were obtained considering the ideal mixture for its components (glycerol and lemon bagasse properties). The boundary conditions used in the simulations of the jacket and polyol domains are showed in **Table 2**.

3. Results and discussion

3.1 Liquefaction yield (LY) and analysis of heat transfer

The experimental results obtained from the three solvent/biomass (s/b) mass ratios are shown in **Table 3**. The experiments started at 25°C and the lateral and the bottom of the reactor walls were at 125°C (due to the vapor steam in the heated jacket). The temperature variation ΔT, in **Table 3**, expresses the average heating rate, for 30 minutes time interval, from time 0(zero) until 90 minutes, for each experiment.

According to data in **Table 3**, the liquefaction yields were influenced by the time of reaction, which is coherent with previous works about other types of biomass [5, 15]. It was observed yields higher than 70 wt% in the three solvent/biomass ratios, for 90 minutes reaction, which are satisfactory results compared to experimental results in literature data [12, 16–18].

Although the highest heating rate (ΔT) was observed in the first 30 minutes (58.6 ± 1.38°C) and followed by the 30-60 minutes interval (9.6 ± 1.83°C), 90 minutes reaction was important to guarantee biomass conversion. It was observed a decrease of the solid residue with time reaction due to the gradual conversion of solid matters into polyol (reduction of 57.91 to 44.46 to 13.48 wt%).

The largest temperature variation occurred in the first 30 minutes due to the high initial gradient temperature between the vessel wall (125.15°C at t = 0 s) and the bulk mixture (25.15 K at t = 0 s). Therefore, at the beginning of liquefaction, it was expected the higher heat transfer rate.

It was also observed that, the higher the amount of glycerol, faster it achieves the final temperature. This behaviour was coherent since the greater the mass of glycerol used (liquid fraction), the higher the thermal conductivity of the mixture (k) and higher the heat transfer rate [19].

Since the steam employed in the liquefaction comes from an autoclave, it was observed a continuous rising of the solution temperature, until it reaches a thermal steady state equilibrium. However, the exchange of thermal energy was limited by

Sample	Time (min)	Temperature (K)	LY (wt%)	ΔT (°C)
Polyol 1	30	356.95	48.63	58.40
	60	366.55	40.41	9.60
	90	369.25	86.52	2.70
Polyol 2	30	357.25	42.09	58.60
	60	367.65	55.54	10.40
	90	369.15	77.62	1.50
Polyol 3	30	360.85	34.27	61.60
	60	367.75	65.79	6.90
	90	370.95	88.37	3.20
	30	361.45	—	62.80
Glycerol	60	367.05	—	5.60
	90	369.15	—	2.10

Table 3.
Experimental results for liquefaction yield (LY) and heating rate (ΔT), according to time reaction and temperatures measured at the vessel.

the heat transfer surface and the combination of the internal thermal resistances, which can be observed through polyol temperature that does not exceed 100°C, due to the physical characteristic of solvent and mixture. This behaviour is coherent with observations of Choi and Mills [20], which showed that apart from the thermal resistance, the tendency of temperature stabilization and its delay may be due to supply energy to promote the endothermic liquefaction reaction.

The knowledge about the evolution of the temperature distribution along the time inside the reactor can be used to estimate the amount of the energy required for the process. The analysis of heat transfer from jacket into the reaction vessel is shown in the following section.

3.2 Computational Fluid Dynamics (CFD) analysis

Despite the superheated vapor flows inside the heated jacket was a steady state simulation, the thermal profiles of polyol mixture were obtained from transient simulation. Therefore, the wall heat flux obtained from jacket domain was used as boundary conditions for polyol domain transient simulations. **Figure 2** shows the simulated results for wall heat flux of jacket domain considering internal surface temperature at 25°C.

According to the profiles presented in **Figure 2**, the wall heat flux from heated jacket domain to reactor vessel domain was not uniform or symmetrical and it was necessary to simulate three-dimensional profiles of fluid velocities and temperature inside the reaction vessel. It was expected that the liquefaction process is affected by temperature, since most of the cases of biomass conversion is well defined by Arrhenius equation [21]. Hence, the evolution in time of the thermal profile behaviour should be related with the evolution in time of the liquefaction yield inside the reaction vessel. However, it worth mentioning that the heated jacket simulation was steady state and the thermal profile in the reactor vessel domain is representative for 90 minutes of operation obtained in a transient simulation. According to the obtained results showed below, this is time enough to the system achieves a natural convection behaviour, able to present a symmetrical

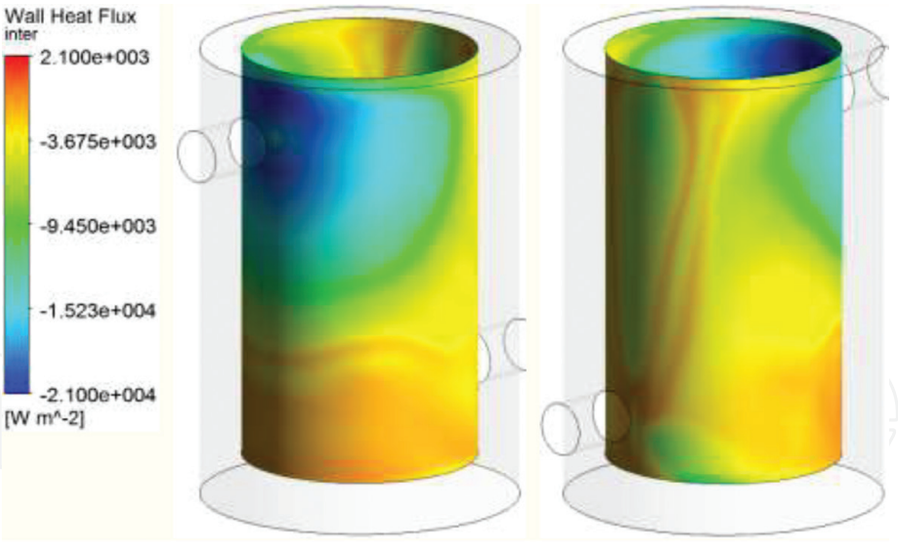

Figure 2.
Wall heat flux profile (W m^{-2}) in the internal surface of the jacket domain visualized by the opposite sides in a semi-isometric view.

profile and significant contribution of conduction mechanism rather than convection in the net heat transfer.

Additionally, in the boundary conditions specifications, it was imported the profile for heat transfer coefficient with external temperature of 125°C. When the temperature near the walls achieves higher values next to 125°C, the effect of the heat flux profile as boundary condition becomes less influent than the specification of fixed temperature and the temperature profile tends to become uniform. Since the temperature gradient drives the heat transfer, it was expected higher heat transfer rates at the beginning of the process, enhanced by convection of momentum and energy, followed by a soft decreasing of its contribution until to establish the temperature profile as the temperature gradient also decreases. Therefore, the heat flux was more influent in the initial time-steps due to the high values of temperature gradient. **Figure 3** presents the evolution of temperature profile inside the liquefaction vessel. It can be seen that the temperature profile becomes stable between 45 and 60 min of heating, considering the reaction vessel without mechanical agitation and the mixtures Polyol 1, 2 and 3. These results are in accordance with those results from experimental analysis, present in **Table 3**.

According to the temperature profiles of **Figure 3**, there was a tendency for occurrence of a natural convection structure after 20 minutes of heating. It also can be observed that high temperatures appear first in the superior part and there was a slow heating from above to below. However, there was a centreline at the vessel axis where the temperatures remain significantly lower than in rest of the domain, due to the downward stream produced by the natural convection cell. After the natural convection structure has been established, it was possible to see that there were two heat fluxes inside the liquefaction vessel. The first was the main (primary) flux with vertical rising streams next to the walls and a descendant stream passing by the reactor axis. The secondary flux, slower than main flux, transports heat predominantly by conduction from the top to the bottom and from axis to walls in radial direction.

The thermal profile for a vertical plane in the two computational domains, vessel and jacket, can be visualized in **Figure 4**. It considered the simulation of Polyol 1, where the thermal profile shown represents the results for steady state jacket domain and for reactor vessel domain at the final time-step (90 min). A simplified

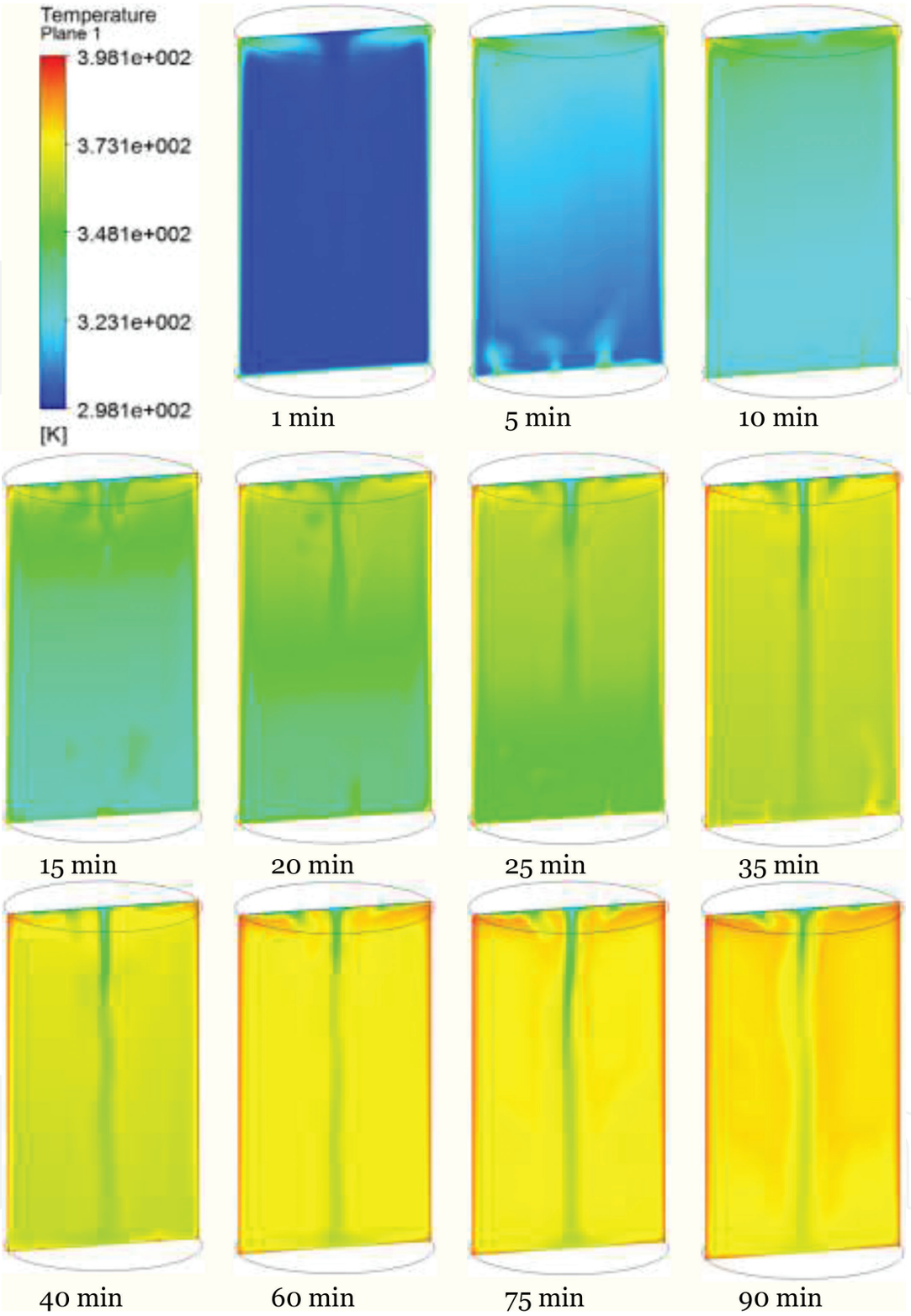

Figure 3.
Time evolution of thermal profile in vertical plane for the glycerol mixture inside the liquefaction vessel.

scheme with the two main heat fluxes, represented by continuous and dashed lines, after the formation of natural heat convection cell is also presented in **Figure 4**.

Despite of the non-uniform profile of wall heat transfer coefficient showed in **Figure 2**, the temperature profile inside liquefaction vessel looked like symmetrical after natural convection has been formed, according to **Figures 3** and **4**. This indicates that, after few minutes of heating, the temperature inside liquefaction vessel becomes more affected by flow pattern than by heat transfer from heated walls.

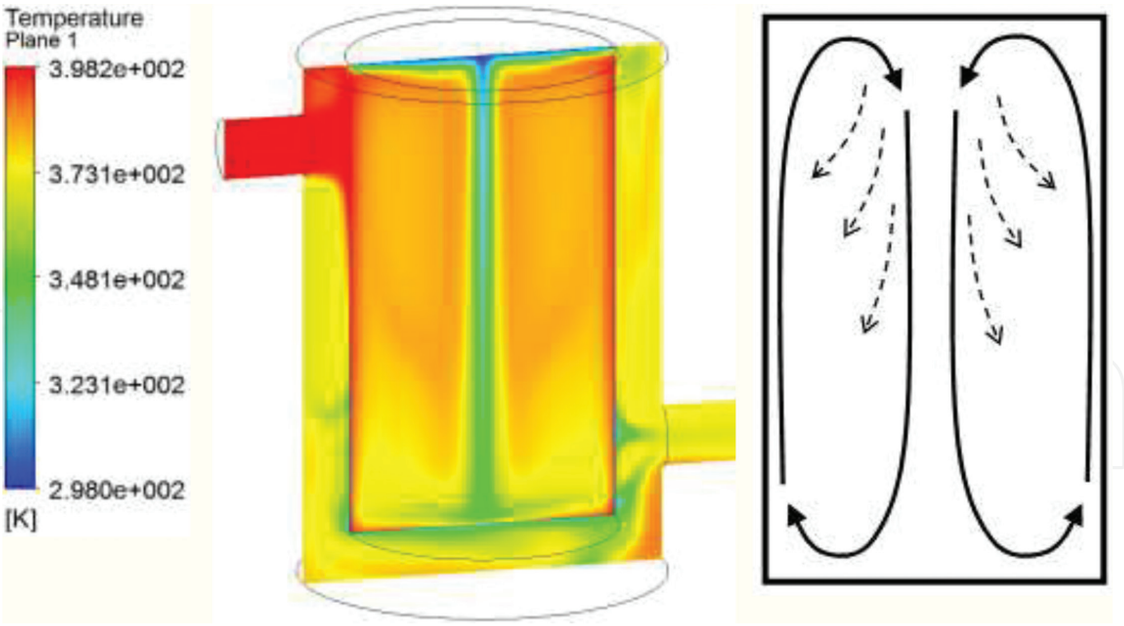

Figure 4.
Thermal profile in vertical plane for the two simulated domains showed simultaneously and the simplified scheme of the primary (continuous) and secondary (dashed) heat fluxes inside reaction vessel after the formation of natural convection cell.

However, it is hard for the hybrid (upwind/central difference) discretization scheme to represent a not imposed symmetry (zero derivative) in the central axis for velocity and temperature [22]. Hence, CFD solver results can presents transient and local instabilities. Therefore, it was expected that the eddy structure of falling cold flow in the axis domain oscillates significantly when the natural convection cell was formed. Since the liquefaction is influenced by temperature, it is convenient to evaluate the evolution of the temperature over the time. Considering that heat transfer occurs through out the walls, it can be expected the lowest temperatures at the centre of reactor vessel axis (0.0, 0.2, 0.0 m), this point was the chosen one to analyse the heating of the polyol mixture.

Despite of the low velocities and high viscosity for the mixture biomass with solvent, the transient temperature values assuming laminar flow at the centre of domain present large oscillation over the time. Using a RANS turbulence model, the vector and scalar variables obtained from CFD simulations could be expressed by a time average according to Reynolds average definitions for velocity components u_i (Eq. (2)) and T (Eq. (3)):

$$u_{i,turb} = U_i = \overline{u}_i = \frac{1}{\Delta t}\int_0^{\Delta t} u_i(t)dt \tag{2}$$

$$T_{turb} = \overline{T} = \frac{1}{\Delta t}\int_0^{\Delta t} T(t)dt \tag{3}$$

Because every value calculated under the turbulent RANS is time averaged, results from models, such as standard k-ε or SST, should present less oscillation than those observed from laminar regime [22]. However, to compare the simulated results with experimental data, those oscillations are still large and should be attenuated. In order to represent the simulated results with less variation, it was employed a moving average in the simulated temperatures (Eq. (4)).

$$T_{mov\,ave,j} = \frac{1}{5}\sum_{j-2}^{j+2} T_{turb,j} \tag{4}$$

Where the subscript j refers to a specific time-step and each $T_{mov\ ave,j}$ is the average temperature value of the five values around of the its determinate time j. The comparison between the experimental data and simulated results, expressed by the moving average temperatures, is presented in **Figure 5**.

According to samples Polyol 1 and 2, there are two different periods of time to be analysed: before 25 minutes and after 25 minutes of heating. In the first period, the experimental temperatures are lower than simulated results and in the second period the experimental values are higher than simulation temperatures. However, this behaviour, that presents two different periods, is not observed for Polyol 3 and the simulated results presented temperatures below the experimental data. Polyol 3 behaves similar to crude glycerol, since it has higher solvent/biomass ratio (**Table 3**).

Due to the liquefaction of solid biomass, the liquid mass increases. This transformation occurs mainly above 30 minutes. From this time, it can be observed that the behaviour of Polyol 1 and 2, started being similar to Polyol 3 (and crude glycerol). Although the polyols have higher density and viscosity compared to crude glycerol [23], the heat changes the fluid properties, which may favour the heat transfer by conduction and natural convection.

Changes in the fluid properties may also be the main reason of the difference between experimental results and CFD simulation, since the model used did not consider dynamic density and viscosity values.

At last, from **Figure 5**, it can be observed the tendency of a flat plateau formation. It has a little variation in temperature between 60 and 90 minutes of heating, which may be an evidence of the stabilization of the system or a period that all supplied energy is consumed to promote the endothermic liquefaction reaction.

In a nutshell, CFD simulations is suitable to represent the experimental data. Although it overestimates the temperatures before 25 minutes of heating for the Polyol 1 and Polyol 2 and underestimates it after 25 minutes of operation, the

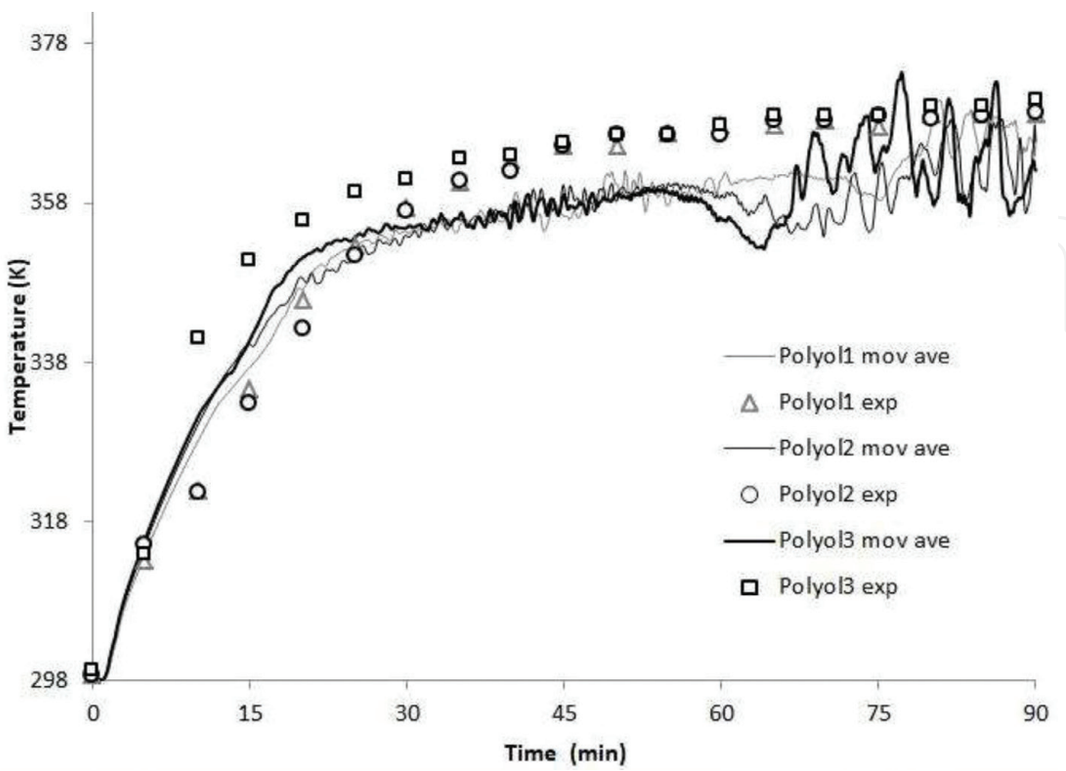

Figure 5.
Evolution in time of temperature: comparison between experimental data (exp) and simulation results treated by moving average (mov ave), for the samples Polyol 1, 2 and 3.

simulation underestimates the temperatures inside the reaction vessel for Polyol 3 during all the time of experiment. It is worth mentioning that several endothermic and exothermic reactions occur during the experiments but the CFD simulations does not consider any chemical reaction neither changes in fluids properties.

4. Conclusion

From the CFD thermal profile, in vertical plane, it was necessary 60 minutes to achieve a steady state of heating in the mixture inside this liquefaction vessel. The model is accordance with experimental data, which shows the heating hate (ΔT) was significant lower in the last stage (60 to 90 minutes). Although, the highest ΔT was observed in the first steps, the 90 minutes reaction was important to guarantee biomass conversion into polyols (LY greater than 77 wt%).

The increase in the temperature of the mixture inside the reactor occurred due to the conduction and natural convection phenomena. These phenomena of heat transfer were favoured by the modification in the proprieties of the fluids, due to the heating of them and due to the reduction of the biomass and formation of the polyol. However, from the experimental data and CFD simulation it was observed that mixture temperature did not exceeded 100°C. The temperature inside the reactor was limited to the thermal conductivity of the system and its reagents.

In conclusion, Computational Fluid Dynamics transient simulations, even presenting some oscillations, can be a satisfactory way to analyse heat transfer in liquefaction process, using crude glycerol as solvent.

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Conflict of interest

The authors declare no conflict of interest.

Author contributions

B.S. Leite and S.A.F. Leite conducted the liquefaction process; D.J.O. Ferreira conducted the CFD analysis; V.F.C. Lins analysed the results and reviewed the paper; all authors had approved the final version.

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References

[1] Hassan EM, Shukry N. Polyhydric alcohol liquefaction of some lignocellulosic agricultural residues. Ind Crops Prod. 2008 Jan;**27**(1):33-38

[2] Ye L, Zhang J, Zhao J, Tu S. Liquefaction of bamboo shoot shell for the production of polyols. Bioresour Technol. 2014;**153**:147-153

[3] Nakano T. Mechanism of Thermoplasticity for Chemically-Modified Wood. Vol. 48, Holzforschung - International Journal of the Biology, Chemistry, Physics and Technology of Wood. 1994. p. 318.

[4] Lee S-H, Yoshioka M, Shiraishi N. Liquefaction of corn bran (CB) in the presence of alcohols and preparation of polyurethane foam from its liquefied polyol. J Appl Polym Sci. 2000 Oct;**78**(2):319-325

[5] Briones R, Serrano L, Llano-Ponte R, Labidi J. Polyols obtained from solvolysis liquefaction of biodiesel production solid residues. Chem Eng J. 2011;**175**(1):169-175

[6] Lee JH, Lee JH, Kim DK, Park CH, Yu JH, Lee EY. Crude glycerol-mediated liquefaction of empty fruit bunches saccharification residues for preparation of biopolyurethane. J Ind Eng Chem. 2016;**34**:157-164

[7] Dimitriadis A, Bezergianni S. Hydrothermal liquefaction of various biomass and waste feedstocks for biocrude production: A state of the art review. Renew Sustain Energy Rev. 2017;**68**(May 2016):113-125

[8] Rafiqul I, Lugang B, Yan Y, Li T. Study on co-liquefaction of coal and bagasse by Factorial Experiment Design Method. Fuel Process Technol. 2000;**68**(1):3-12

[9] Cao L, Zhang C, Hao S, Luo G, Zhang S, Chen J. Effect of glycerol as co-solvent on yields of bio-oil from rice straw through hydrothermal liquefaction. Bioresour Technol. 2016;**220**:471-478

[10] Li H, Feng S, Yuan Z, Wei Q, Xu CC. Highly efficient liquefaction of wheat straw for the production of bio-polyols and bio-based polyurethane foams. Ind Crops Prod. 2017 Dec;**109**:426-433

[11] Leite SAF, Leite BS, Carriço CS, Rosa YG, Figueiredo MTD. Biopolyol and Foam Production From Lemon Bagasse Liquefaction. 2018;**65**:376-381

[12] Carriço CS, Fraga T, Pasa VMD. Production and characterization of polyurethane foams from a simple mixture of castor oil, crude glycerol and untreated lignin as bio-based polyols. Eur Polym J. 2016;**85**:53-61

[13] Lamb J. Influence of water on the thermal properties of foods. Chem Ind. 1976;**24**:1046

[14] Renaud T. Mesure et modélisation de la conductivité et de la diffusivité thermiques des produits alimentaires congelés et non congelés. 1990.

[15] Juhaida MF, Paridah MT, Mohd. Hilmi M, Sarani Z, Jalaluddin H, Mohamad Zaki AR. Liquefaction of kenaf (*Hibiscus cannabinus* L.) core for wood laminating adhesive. Bioresour Technol. 2010 Feb;101(4):1355-60.

[16] Hejna A, Kirpluks M, Kosmela P, Cabulis U, Haponiuk J, Piszczyk Ł. The influence of crude glycerol and castor oil-based polyol on the structure and performance of rigid polyurethane-polyisocyanurate foams. Ind Crops Prod. 2017 Jan;**95**:113-125

[17] Hu S, Li Y. Polyols and polyurethane foams from base-catalyzed liquefaction of lignocellulosic biomass by crude glycerol: Effects of crude glycerol

impurities. Ind Crops Prod [Internet]. 2014 Jun 1 [cited 2018 Jun 26];57:188-94. Available from: https://www.sciencedirect.com/science/article/pii/S0926669014001666

[18] Kairytė A, Vėjelis S. Evaluation of forming mixture composition impact on properties of water blown rigid polyurethane (PUR) foam from rapeseed oil polyol. Ind Crops Prod. 2015 Apr;**66**:210-215

[19] Smith JM, Van Ness HC, Abbott MM, Swihart MT. Introduction to Chemical Engineering Thermodynamics. 8th ed. Education M-HH, editor. 2017. 768 p.

[20] Choi H, Mills AF. Heat and mass transfer in metal hydride beds for heat pump applications. Int J Heat Mass Transf. 1990 Jun;33(6):1281-8.

[21] Syed AH. CFD modeling for direct liquefaction of biomass in hydrothermal media [Internet]. Norwegian University of Science and Technology; 2013. Available from: https://core.ac.uk/reader/52098590

[22] Versteeg HK, Malalasekera W. Computational Fluid Dynamics – The Finitie Volume Method. 2nd ed. Pearson; 2007. 503 p.

[23] Leite BS, Ferreira DJO, Leite SAF, Bastos FS, Lins VFC, Castro BT. Investigation of Agricultural Biomass Residues in Liquefaction Process. 2019;10(11).